



chain nodes :

37	38	39	40	41	42	44	45	47	48	50	51	52	53	55	56	57	58
60	64	65															

ring nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
22	23	24	25	26	27	28	29	30	31	32	33	34	35	36						

ring/chain nodes :

59

chain bonds :

5-37	7-64	9-37	11-38	14-38	17-39	18-50	19-41	22-40	23-55	25-65
27-41	29-42	32-42	37-44	38-45	39-40	41-47	42-48	50-51	50-52	
50-53	55-56	55-57	55-58							

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	7-8	7-12	8-9	9-10	10-11	11-12	13-14
13-18	14-15	15-16	16-17	17-18	19-20	19-24	20-21	21-22	22-23			
23-24	25-26	25-30	26-27	27-28	28-29	29-30	31-32	31-36	32-33			
33-34	34-35	35-36										

exact/norm bonds :

5-37	7-64	9-37	11-38	14-38	18-50	19-41	23-55	25-65	27-41	29-42
32-42	37-44	38-45	41-47	42-48	50-51	50-52	50-53	55-56	55-57	
55-58										

exact bonds :

17-39	22-40	39-40								
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normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6	7-8	7-12	8-9	9-10	10-11	11-12	13-14
13-18	14-15	15-16	16-17	17-18	19-20	19-24	20-21	21-22	22-23			
23-24	25-26	25-30	26-27	27-28	28-29	29-30	31-32	31-36	32-33			
33-34	34-35	35-36										

isolated ring systems :

containing 1 : 13 : 1 25 : 31 :

G1:H, CH3

G2:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
34:Atom 35:Atom 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS 44:CLASS 45:CLASS 47:CLASS 48:CLASS 50:CLASS
51:CLASS 52:CLASS 53:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 64:CLASS 65:CLASS